

Theory of magnetic excitations in the Kondo lattice

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We present a theory for the spin excitations of the Kondo lattice. We derive an effective Hamiltonian, which describes Fermionic spin 1/2 charge fluctuations interacting with Bosonic triplet spin fluctuations. Evaluating the polarization bubble in the magnon Green's function with the free charge excitation's Green's function gives a quantitative description of the 'spin gap' and 'charge gap' as obtained from numerical calculations for the Kondo insulator.

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The Kondo lattice model is a generic model of strongly correlated electrons. It may be applicable, with some variations, to a wide variety of materials, most notably the Heavy Fermion metals [1,2] and Kondo insulators [3]. It is the purpose of the present manuscript to present a conceptually very simple theory for the spin and charge excitations of this model, and their mutual interplay. The basic idea is, in the spirit of the cell-perturbation theory developed by Jefferson and co-workers [4], to split the systems up into sub-units which can be solved exactly. Coupling the sub-units together leads to a simple effective Hamiltonian. As has been shown in Refs. [5] for the one particle-spectra and as will be shown in the present work for the spin excitations, solving this Hamiltonian with the simplest approximations possible produces already quite satisfactory results. An approach which is similar in spirit has been proposed for the Kondo lattice by Pérez-Conde *et al.* [6] and for the description of π -electrons in conjugated polymers by Pleutin [7]. The Hamiltonian considered in this work reads

$$H_{sc} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + J \sum_n \mathbf{S}_{n,c} \cdot \mathbf{S}_{n,f}. \quad (1)$$

Here $\epsilon_{\mathbf{k}} = \sum_n \exp(i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_m)) t_{mn}$ is the Fourier transform of the hopping integral t_{nm} for the c electrons, and $\mathbf{S}_{n,c}$ ($\mathbf{S}_{n,f}$) denotes the spin operator for conduction electrons (f -electrons) in cell n . A unit cell contains one c -orbital and one localized spin.

The physical parameter regime is $J < \max |t_{nm}|$. It was shown previously [5], however, that an 'expansion' around the limiting case $t_{mn}=0$, where the ground state for one conduction electron/unit cell is simply a product of single-cell singlets, gives in fact a surprisingly good description even in the physical parameter regime. The basic idea is a mapping between a suitably restricted Hilbert space and states of effective Fermions which basically stand for charge fluctuations in the singlet background. More precisely, when a single cell is in the two-electron singlet state, we consider this cell to be empty. If the cell n is occupied only by the f -spin we consider it occupied by a hole-like Fermion, created by $a_{n,\sigma}^\dagger$, if it is occupied by three electrons we model this by the pres-

ence of an electron-like Fermion, created by $b_{n,\sigma}^\dagger$. So far our 'translation table' thus reads:

$$\begin{aligned} |vac\rangle &\rightarrow \frac{1}{\sqrt{2}} (c_{n,\uparrow}^\dagger f_{n,\downarrow}^\dagger - c_{n,\downarrow}^\dagger f_{n,\uparrow}^\dagger) |0\rangle, \\ a_{n,\sigma}^\dagger |vac\rangle &\rightarrow f_{n,\sigma}^\dagger |0\rangle, \\ b_{n,\sigma}^\dagger |vac\rangle &\rightarrow c_{n,\uparrow}^\dagger c_{n,\downarrow}^\dagger f_{n,\sigma}^\dagger |0\rangle. \end{aligned} \quad (2)$$

In the reduced Hilbert space which is built up from product states of single cell states of the type (2), the Hamiltonian (1) takes the form [5]

$$\begin{aligned} H_{eff} = & \frac{1}{2} \sum_{\mathbf{k},\sigma} [(-\epsilon_{\mathbf{k}} + \frac{3J}{2}) a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma} + (\epsilon_{\mathbf{k}} + \frac{3J}{2}) b_{\mathbf{k},\sigma}^\dagger b_{\mathbf{k},\sigma}] \\ & - \frac{1}{2} \sum_{\mathbf{k},\sigma} \text{sign}(\sigma) \epsilon_{\mathbf{k}} (b_{\mathbf{k},\sigma}^\dagger a_{-\mathbf{k},\bar{\sigma}}^\dagger + H.c.). \end{aligned} \quad (3)$$

The Fermions have to obey a hard-core constraint, i.e. no cell may be occupied by more than one Fermion. This constraint is necessary to make sure that the state of any given cell be unique. If to simplest approximation we relax this constraint, the Hamiltonian (3) can be solved by Bogoliubov transformation. Introducing $\Delta=3J/2$, the quasiparticle dispersion [5] is

$$E_{\pm}(\mathbf{k}) = (1/2) [\epsilon_{\mathbf{k}} \pm \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}], \quad (4)$$

with the resulting quasiparticles

$$\begin{aligned} \gamma_{\mathbf{k},-,\sigma} &= u_{\mathbf{k}} b_{\mathbf{k},\sigma} + \text{sign}(\sigma) v_{\mathbf{k}} a_{-\mathbf{k},\bar{\sigma}}^\dagger, \\ \gamma_{\mathbf{k},+,\sigma} &= -v_{\mathbf{k}} b_{\mathbf{k},\sigma} + \text{sign}(\sigma) u_{\mathbf{k}} a_{-\mathbf{k},\bar{\sigma}}^\dagger, \end{aligned} \quad (5)$$

The choice of signs ensures that e.g. $[S^+, \gamma_\uparrow] = -\gamma_\downarrow$. The Hamiltonian (3) operates only within a reduced Hilbert space. Any states where a unit cell with two electrons (one f and one c -electron) is in the *triplet* state are projected out. This restriction makes the propagation of the charge fluctuations γ^\dagger completely coherent, and is justified to some degree by the quite good agreement of the resulting single-particle spectra with Lanczos diagonalization [5] - but ultimately it is of course an uncontrolled approximation. Therefore we now want to

enlarge the Hilbert space to its full size by introducing an additional effective particle \mathbf{t}_i , whose presence in a given cell i implies that this cell is occupied by two electrons in the triplet state. Since the three components of a triplet are isomorphic to a 3-vector, \mathbf{t}_i must be a vector particle. We thus enlarge the ‘translation table’ (2) by

$$\mathbf{t}_n^\dagger |vac\rangle \rightarrow 2i\sqrt{2} c_{n,\tau}^\dagger (\boldsymbol{\sigma}\boldsymbol{\sigma}^y)_{\tau,\tau'} f_{n,\tau'}^\dagger |0\rangle, \quad (6)$$

where $\boldsymbol{\sigma}$ is the vector of Pauli matrices (with $\sigma^2=3/4$) and repeated spin indices τ, τ' are summed over.

The quantum numbers of the \mathbf{t}^\dagger particle are spin 1 and charge 0, whence it must be a Boson. As was the case for the Fermions, the Bosons have to obey a mutual exclusion principle, i.e. no two particles, of either Fermionic or Bosonic nature, must occupy the same site.

Having introduced the \mathbf{t}^\dagger Bosons to mark spin excited cells, we proceed to derive the Hamiltonian which describes their interaction with the charged excitations a^\dagger and b^\dagger . Figure 1 gives a survey of the different interaction

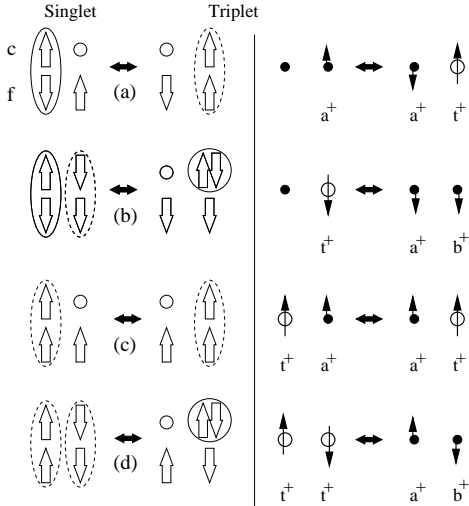


FIG. 1. Different hopping processes which involve triplet cells (left panel) and their representation in terms of book-keeping Fermions and Bosons (right panel). The transition is always accomplished by the hopping of a physical \uparrow -electron from left to right. Spin and site labels on the book-keeping particles in the left panel are suppressed for simplicity.

processes that are possible. The form of the respective terms in the Hamiltonian can be inferred from the requirement of Hermiticity, spin rotation and time reversal invariance. The first type of interaction process we consider involves two Fermion operators and one Boson operator. They correspond first to the emission (or absorption) of a triplet as a charge fluctuation hops from one cell into the other (see Figure 1a). Another process of this type is the pair creation of one electron-like and

one hole-like charge fluctuation in which a triplet is annihilated (see Figure 1b). The only way to construct a spin scalar from two spinors (say: a^\dagger and a) and one vector (\mathbf{t}^\dagger) is to first couple the spinors into a vector:

$$\begin{aligned} S_{mn}^a &= a_{m,\tau}^\dagger \boldsymbol{\sigma}_{\tau,\tau'} a_{n,\tau'}, \\ S_{mn}^b &= b_{m,\tau}^\dagger \boldsymbol{\sigma}_{\tau,\tau'} b_{n,\tau'}, \\ S_{mn}^+ &= 2ib_{m,\tau}^\dagger (\boldsymbol{\sigma}\boldsymbol{\sigma}^y)_{\tau,\tau'} a_{n,\tau'}^\dagger, \end{aligned} \quad (7)$$

and then form its scalar product with the vector \mathbf{t}^\dagger . Due to the product nature of the basis states, the matrix elements can be evaluated by considering just two cells m and n connected by the hopping integral t_{mn} [5]. The result is:

$$\begin{aligned} H_1 &= \sum_{m,n} t_{mn} [\mathbf{t}_m \cdot (\mathbf{S}_{mn}^a - \mathbf{S}_{mn}^b) \\ &\quad + (\mathbf{t}_m - \mathbf{t}_n) \cdot \mathbf{S}_{mn}^+] + H.c. \end{aligned} \quad (8)$$

Next, we consider processes involving two Fermions and two Bosons. Examples are shown in Figure 1c, where a triplet and a charge fluctuation exchange their position, and in Figure 1d, where two triplets are annihilated in the pair creation of one electron-like and one hole-like charge fluctuation. There are two ways to form a spin scalar from two spinors and two vectors: first, one can contract both the spinors and the vectors separately into scalars and multiply these. This term describes processes where the Fermion and the Boson exchange their position without exchanging spin. Alternatively, one can combine the two spinors into a vector following (7), and form the wedge product of the three resulting vectors. We thus find the additional terms

$$\begin{aligned} H_2 &= \sum_{m,n} \frac{t_{mn}}{2} \mathbf{t}_m^\dagger \cdot \mathbf{t}_n \sum_{\sigma} (b_{n,\sigma}^\dagger b_{m,\sigma} - a_{m,\sigma}^\dagger a_{n,\sigma}) + \\ &\sum_{m,n} [\frac{t_{mn}}{2} \mathbf{t}_m^\dagger \cdot \mathbf{t}_n \sum_{\sigma} \text{sign}(\sigma) b_{n,\sigma}^\dagger a_{m,\sigma} + H.c.] \\ H_3 &= i \sum_{m,n} t_{mn} (\mathbf{S}_{mn}^a - \mathbf{S}_{mn}^b) \cdot (\mathbf{t}_n^\dagger \times \mathbf{t}_m) \\ &+ i \sum_{m,n} [t_{mn} \mathbf{S}_{mn}^+ \cdot (\mathbf{t}_n^\dagger \times \mathbf{t}_m^\dagger) + H.c.] \end{aligned} \quad (9)$$

The terms H_1 , H_2 and H_3 combined describe all possible interactions of the vector Bosons with the Fermionic charge fluctuations. The only term still missing to complete the Hamiltonian is the ‘energy of formation’ of the triplets: $H_4 = J \sum_n \mathbf{t}_n^\dagger \cdot \mathbf{t}_n$.

Having written down the Hamiltonian we proceed to investigate the physics resulting from it. For simplicity we restrict ourselves in this paper to the case of half-filling, i.e. the ‘Kondo insulator’. As our overall guideline we try to keep the approximations involved as simple as possible and consequently neglect the 4-particle vertices H_2 and H_3 . This leaves us with H_1 , which describes the propagation of a triplet by an RKKY-like process: the triplet

may be converted into an electron-hole pair, which may later recombine at another site. Alternatively, it may be absorbed by an electron-like or hole-like charge fluctuation, and be re-emitted at a different site. After Fourier and Bogoliubov transformation of H_1 :

$$H_1 = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}, \mathbf{k}} \sum_{\mu, \nu = \pm} M_{\mathbf{k}, \mathbf{q}}^{\mu, \nu} t_{\mathbf{q}}^{\dagger} \cdot \gamma_{\mathbf{k}, \mu, \tau}^{\dagger} \sigma_{\tau, \tau'} \gamma_{\mathbf{k}+\mathbf{q}, \nu, \tau'},$$

$$M_{\mathbf{k}, \mathbf{q}}^{-, -} = \epsilon_{\mathbf{k}+\mathbf{q}} v_{\mathbf{k}} (v_{\mathbf{k}+\mathbf{q}} - u_{\mathbf{k}+\mathbf{q}}) - \epsilon_{\mathbf{k}} u_{\mathbf{k}+\mathbf{q}} (u_{\mathbf{k}} - v_{\mathbf{k}}),$$

$$M_{\mathbf{k}, \mathbf{q}}^{-, +} = \epsilon_{\mathbf{k}+\mathbf{q}} v_{\mathbf{k}} (v_{\mathbf{k}+\mathbf{q}} + u_{\mathbf{k}+\mathbf{q}}) + \epsilon_{\mathbf{k}} v_{\mathbf{k}+\mathbf{q}} (u_{\mathbf{k}} - v_{\mathbf{k}}),$$

$$M_{\mathbf{k}, \mathbf{q}}^{+, -} = \epsilon_{\mathbf{k}+\mathbf{q}} u_{\mathbf{k}} (v_{\mathbf{k}+\mathbf{q}} - u_{\mathbf{k}+\mathbf{q}}) + \epsilon_{\mathbf{k}} u_{\mathbf{k}+\mathbf{q}} (u_{\mathbf{k}} + v_{\mathbf{k}}),$$

$$M_{\mathbf{k}, \mathbf{q}}^{+, +} = \epsilon_{\mathbf{k}+\mathbf{q}} u_{\mathbf{k}} (v_{\mathbf{k}+\mathbf{q}} + u_{\mathbf{k}+\mathbf{q}}) - \epsilon_{\mathbf{k}} v_{\mathbf{k}+\mathbf{q}} (u_{\mathbf{k}} + v_{\mathbf{k}}),$$

we introduce the triplet Green's function (where α may be x, y or z):

$$D(\mathbf{q}, \omega) = -i \langle T t_{\mathbf{q}, \alpha}^{\dagger} t_{\mathbf{q}, \alpha} \rangle$$

$$= \lim_{\epsilon \rightarrow 0^+} \frac{1}{\omega - J - \Sigma(\mathbf{q}, \omega) + i\epsilon}. \quad (10)$$

For the self-energy $\Sigma(\mathbf{q}, \omega)$ we choose the simplest diagram possible, i.e. the polarization bubble in Figure 2.

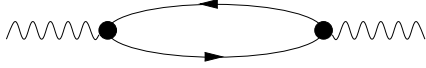


FIG. 2. The self-energy $\Sigma(\mathbf{q}, \omega)$ used for the calculation of the triplet dispersion (the wiggly triplet legs to the right and left must be removed).

The result is:

$$\Sigma(\mathbf{q}, \omega) = \frac{-i}{2N} \sum_{\mathbf{k}} \sum_{\mu, \nu = \pm} |M_{\mathbf{k}, \mathbf{q}}^{\mu, \nu}|^2$$

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} G_{\nu}(\mathbf{k} + \mathbf{q}, \omega' + \omega) G_{\mu}(\mathbf{k}, \omega'),$$

$$G_{\mu}(\mathbf{k}, \omega') = \frac{\delta_{\mu, -}}{\omega - E_{-}(\mathbf{k}) - i\epsilon} + \frac{\delta_{\mu, +}}{\omega - E_{+}(\mathbf{k}) + i\epsilon} \quad (11)$$

(we are using the free Green's function $G_{\mu}(\mathbf{k}, \omega')$ for the charge fluctuations γ^{\dagger}).

To describe the low energy scales of the Kondo lattice at least approximately, we still have to deal with the constraints. We thereby follow Gopalan *et al.* [10] and use a simple mean-field like renormalization of the hopping integral. We consider the vacuum state, where each site is occupied by a singlet, as a condensate of an additional Bosonic particle, s_n^{\dagger} , which stands for to the two-electron singlet state. Then, in the Fermionic Hamiltonian (3) and in th ertem H_1 we have to replace

$$b_{m, \sigma}^{\dagger} a_{n, \sigma}^{\dagger} \rightarrow (b_{m, \sigma}^{\dagger} s_m) (a_{n, \sigma}^{\dagger} s_n),$$

$$a_{m, \sigma}^{\dagger} a_{n, \sigma} \rightarrow (a_{m, \sigma}^{\dagger} s_m) (s_n^{\dagger} a_{n, \sigma}),$$

$$\mathbf{t}_m \cdot \mathbf{S}_{mn}^a \rightarrow s_n^{\dagger} \mathbf{t}_m \cdot \mathbf{S}_{mn}^a$$

(and analogously for the other terms). The constraint takes the form

$$s_n^{\dagger} s_n + \sum_{\sigma} (a_{n, \sigma}^{\dagger} a_{n, \sigma} + b_{n, \sigma}^{\dagger} b_{n, \sigma}) + \mathbf{t}_n^{\dagger} \cdot \mathbf{t}_n = 1.$$

We now assume that the s^{\dagger} singlet is condensed [10], so that the respective operators can be replaced by the real number s which is determined from

$$s^2 = 1 - \sum_{\sigma} (a_{n, \sigma}^{\dagger} a_{n, \sigma} + b_{n, \sigma}^{\dagger} b_{n, \sigma}) \quad (12)$$

(this means that we neglect the density of triplets, $\sum_n \mathbf{t}_n^{\dagger} \cdot \mathbf{t}_n$, which is a good approximation for large and moderate values of J). All in all, in the Hamiltonian (3) we then have to replace throughout $\epsilon_{\mathbf{k}} \rightarrow s^2 \epsilon_{\mathbf{k}}$, whereas H_1 changes according to $H_1 \rightarrow s H_1$.

Figure 3 then shows the calculated triplet spectral density, $A(\mathbf{q}, \omega) = \Im(1/\pi) D(\mathbf{q}, \omega)$. This shows one dominant magnetic excitation, wich has quite a substantial dispersion of order J . Such a sharp low-energy mode which appears only in the spin correlation function has also been observed in Quantum Monte-Carlo simulations at low temperatures [8]. Near $q=\pi$ the dispersion takes its minimum and thus defines the 'spin gap', Δ_s , i.e. the lowest energy required to create a magnetic excitation out of the ground state. Also shown in Figure 3 is the dispersion of the two single particle bands, $E_{\pm}(k)$. Were

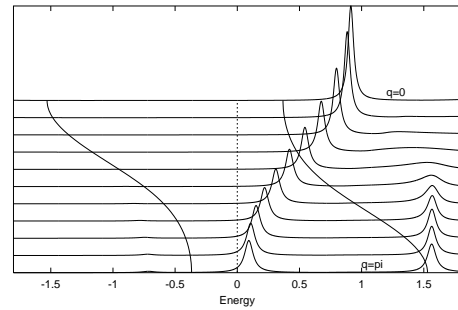


FIG. 3. Triplet spectral density $A(\mathbf{q}, \omega)$ for the 1D Kondo lattice with $J/t=1.0$, as a function of frequency and momentum. The Lorentzian broadening $\epsilon=0.05$.

it not for the low-energy triplet mode, the lowest possible excitation would correspond to exciting one Fermion from the occupied band into the unoccupied one. The energy required for this is the so-called quasiparticle gap $\Delta_{QP} = E_{-}(k=\pi) - E_{+}(k=0)$. If the interaction between the particle-hole pair created in this way is small, this energy should also correspond to the so-called charge gap Δ_c , the energy of the lowest excitation observable in

the density correlation function. In fact, density matrix renormalization group (DMRG) calculations by Yu and White [9] have shown that this neglect of interaction is quite a good approximation. To check our theory, we can thus compare the quasiparticle gap $\Delta_{QP} \approx \Delta_c$ and the spin gap, Δ_s , to the results of Yu and White. This is done in Figure 4 for different values of the Kondo exchange J . The gaps Δ_{QP} and Δ_s differ strongly - as is to be expected because they correspond to completely different types of excitations, i.e. the transfer of a charge fluctuation from the lower to the upper band on one hand, and the propagating triplet on the other. For $J/t \geq 1$ the agreement between theory and numerics is quantitative - this demonstrates that even our very simple and

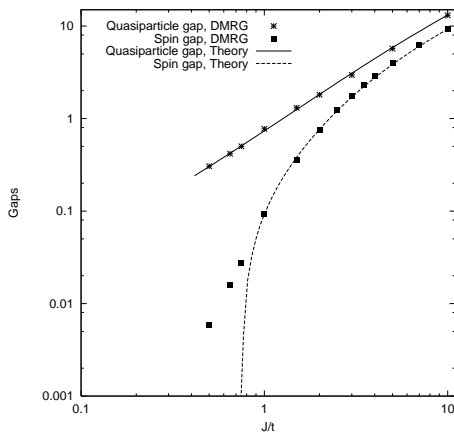


FIG. 4. Comparison of spin gap and quasiparticle gap in the 1D Kondo lattice as obtained by Yu and White [9] from DMRG calculations on a chain with 24 sites to the results of the present theory.

non-selfconsistent calculation of the Green's function apparently captures the essential physics. For small values of J our present approximation is not to be trusted any longer. The main reason is that for small J/t the probability for charge fluctuations becomes very large (J sets the energy scale for the pair-breaking energy) whence our mean-field approximation (12) predicts a quite dramatic renormalization of $\epsilon_{\mathbf{k}}$ - such a renormalization, however, is not observed in Lanczos calculations [5]. Surprisingly enough, Figure 4 shows that despite this problem the estimate for the quasiparticle gap remains accurate even for small J/t - this agreement, however, may as well be fortuitous.

In summary, we have derived a theory for the dynamics of spin and charge excitations in the Kondo lattice and their interaction. The 'purely Fermionic' version, i.e. excluding the spin excitations, has recently been shown to give quite good results when compared to Lanczos di-

agonalization, as a matter of fact for a wide variety of different versions of the Kondo lattice [5]. Augmenting the formalism by Bosonic spin excitations and using the simplest approximations possible, i.e. a mean-field approximation to deal with the constraint and a lowest order evaluation of the Fermionic polarization bubble, we could obtain also a quite satisfactory description of the spin dynamics. In particular, at least for moderate values of the Kondo exchange J , a quantitative description of the spin and charge gap as inferred from DMRG calculations was possible. This gives reason for some optimism to create, mainly by using more sophisticated methods to deal with the constraint [11] in the case of small J/t , a theory which is capable of describing the Kondo lattice from the largest energy scales (i.e. those of the Hubbard bands) down to the smallest ones (i.e. the spin gap). It should also be noted that the formalism is independent of dimensionality or lattice geometry. It involves comparatively little numerical effort and is therefore not restricted either to the somewhat 'toy model type' systems considered so far. In fact, both the quasiparticle dispersion and the self-energy for the spin excitations involve only the unhybridized conduction band dispersion $\epsilon_{\mathbf{k}}$. Using here the results from a 'frozen core' LDA band structure calculation may allow to apply the present formalism rather directly to quite realistic systems. I would like to thank Dr. C. C. Yu and Dr. S. R. White for providing me with the data from Ref. [9].

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